Development of Numerical and Analytical Solutions forHeat Transfer Analysis of Composite Medium and its Applications

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Heat transfer is the study of thermal energy transport within a medium or among neighbouring media by molecular interaction, fluid motion, and electro-magnetic waves, resulting from a spatial variation in temperature. This variation in temperature is governed by the principle of energy conservation, which when applied to a control volume or a control mass, states that the sum of the flow of energy and heat across the system, the work done on the system, and the energy stored and converted within the system, is zero. A thermal system contains matter or substance and this substance may change by transformation or by exchange of mass with the surroundings.

Multilayered components are extensively utilized in current engineering applications due to the additional advantage of combining physical, mechanical, and thermal properties of several materials. Many of these applications, including structural design, industrial furnaces, nuclear reactors, turbines, rockets, spacecraft, and high-tech devices and instruments, necessitate a detailed knowledge of transient temperature and heat-flux distribution within component layers. Analytical or numerical methods can be used to derive a time-dependent temperature distribution in such components. Nonetheless, numerical solutions are favored and used in practice because analytical methods are either unavailable or have a higher computational complexity. When available, exact solutions are more illuminating than numerical solutions in terms of assessing the governing physics of the situation. Nowadays, such solutions also find their applications in validating and comparing various numerical algorithms, which may help improve computational efficiency of computer codes that currently rely on numerical techniques.

1. Basic Terminology

Material Classification

The materials are classified depending upon their transport properties like thermal conductivity, thermal diffusivity etc as isotropic, anisotropic, and orthotropic.

- **Isotropic material:** Solids which have transport properties that do not depend on direction are said to be isotropic.

Properties:

- The thermal conductivity remains the same in all the directions.
- The heat flux is directly proportional to the temperature gradient at that position.
- The heat flux vector is normal to the isothermal surface passing through that position.

❖ **Anisotropic material:** Solids that have properties exhibit directional characteristics are said to be anisotropic.

Properties:

- The thermal conductivity is not same in all the directions.
- The heat flux is not simply proportional to the temperature gradient, each of the components the temperature is weighted according to the anisotropy of the particular material.
- The heat flux vector is not normal to the surface and it is not parallel to the temperature gradient.

❖ **Orthotropic material:** Solids that have properties completely defined in terms of three perpendicular directions. Those three principal material directions are usually defined by a user defined coordinate system or a user defined reference plane.

It is a particular case of anisotropic material.

Heat Transfer Mechanisms

Heat can be transferred in three different modes: Conduction, Convection, and Radiation. All modes of heat transfer require the existence of temperature difference and all the modes are from high temperature medium to a lower temperature one.

❖ **Conduction:** Conduction is the transfer of energy from the more energetic particles of a substance to the adjacent less energetic ones as a result of interactions between the particles. Conduction can take place in solids, liquids, or gases.

According to French mathematician ***Jean Baptiste Joseph Fourier*** (1768-1830), the heat flux vector is proportional to the temperature gradient, that is,

$$\bar{q}(\bar{r},t) = -k\ \nabla T(\bar{r},t)$$

where, $\bar{q}(\bar{r},t)$ is the heat flux vector and

$\nabla T(\bar{r},t)$ is the temperature gradient vector,

the minus sign is introduced in order to make the heat flow a positive quantity,

the proportionality factor k is called the thermal conductivity of the material having unit *W/mK*.

- **Convection:** Convection is the mode of energy transfer between a solid surface and the adjacent liquid or gas that is in motion. The faster the fluid motion, the grater the convection heat transfers.

  The rate of convection heat transfer is proportional to the temperature difference, and it is expressed by ***Newton's law of cooling*** (1642 -1727),

$$\bar{q}.\bar{n} = h.(T - T_a)$$

  where, $\bar{n}$ is the unit outward normal to the surface and

  T is the surface temperature,

  T_a is the temperature of the fluid sufficiently away from the surface,

  h is the convection heat transfer coefficient in W/m^2K.

- **Radiation:** Radiation is the energy emitted by matter in the form of electromagnetic waves as a result of change in electronic configuration of the atoms or molecules. All the bodies above absolute zero temperature emit thermal radiation.

  The maximum rate of radiation that can be emitted form a surface at thermodynamic temperature T is given by the ***Stefan Boltzmann law*** as,

$$\bar{q}_{\max} = \sigma T^4$$

  where, $\sigma = 5.67 \times 10^{-8}$ W/m^2K^4 is the Stefan Boltzmann constant.

2. Mathematical Formulation

The Differential Equation of Heat Conduction

The differential equation of heat conduction for stationary, homogeneous and isotropic solid with heat generation within the body is given as,

$$\rho c_p \frac{\partial T(\underline{r}, t)}{\partial t} = k \nabla \underline{T}(\underline{r}, t) + g(\underline{r}, t)$$

where, ρ is the density of the solid,

c_p is the specific heat and

$g(\bar{r}, t)$ is the heat generation function of both position and time.

k is the thermal conductivity of a material.

Special cases

- Thermal conductivity is uniform, that is, independent of position and temperature.

$$\frac{1}{\alpha}\frac{\partial T\left(\bar{r},t\right)}{\partial t} = \nabla^2 T\left(\bar{r},t\right) + \frac{g\left(\bar{r},t\right)}{k}$$

where, α is called thermal diffusivity of the medium and is defined as,

$$\alpha = \frac{k}{\rho c_p}$$

- Uniform thermal conductivity, no heat sources.

$$\frac{1}{\alpha}\frac{\partial T\left(\bar{r},t\right)}{\partial t} = \nabla^2 T\left(\bar{r},t\right)$$

which is called as the ***Fourier equation*** of heat conduction or the diffusion equation.

- Uniform thermal conductivity, steady state, heat generation within the solid.

$$\nabla^2 T\left(\bar{r}\right) + \frac{g\left(\bar{r}\right)}{k} = 0$$

which is ***Poisson's equation*.**

- Steady state no heat generation.

$$\nabla^2 T\left(\bar{r}\right) = 0$$

which is ***Laplace equation*.**

In different coordinate systems, the three dimensional, homogeneous differential equation of heat conduction with no heat generation within the solid are given as:

- **In Cartesian coordinate system:**

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$$

where, $T \equiv T(x, y, z, t)$

- **In Cylindrical coordinate system:**

$$\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r} + \frac{1}{r^2}\frac{\partial^2 T}{\partial \phi^2} + \frac{\partial^2 T}{\partial z^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$$

where, $T \equiv T(r, \phi, z, t)$

❖ **In Spherical coordinate system:**

$$\frac{\partial^2 T}{\partial r^2} + \frac{2}{r}\frac{\partial T}{\partial r} + \frac{1}{r^2 \sin\psi}\frac{\partial}{\partial \psi}\left(\sin\psi \frac{\partial T}{\partial \psi}\right) + \frac{1}{r^2 \sin^2 \psi}\frac{\partial^2 T}{\partial \phi^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$$

where, $T \equiv T(r, \psi, \phi, t)$

3. The Boundary Conditions

The differential equation of heat conduction will have numerous solutions unless a set of boundary conditions and initial condition are prescribed. For convenience the linear boundary conditions are separated into three groups:

❖ **Boundary conditions of first kind**

Temperature is prescribed along the boundary surface and for the general case it is a function of both time and position. Special cases include temperature at the boundary is a function of position only or a function of time only or a constant.

If the temperature at the boundary surface vanishes i.e. $T=0$, on the boundary surface s_i.

This special case is called as the homogeneous boundary condition of first kind. A boundary surface which is kept at constant temperature T_o, also a boundary condition of first kind.

Moreover called as the **Dirichlet boundary condition**, named after Johann Peter Gustav Lejeune Dirichlet (1805–1859).

❖ **Boundary conditions of second kind**

The normal derivative of temperature is prescribed at the boundary surface it may be a function of both time and position. For a boundary surface that fits the coordinate surface of the orthogonal coordinate system it is given in the form,

$$\frac{\partial T}{\partial n_i} = f_i\left(r_s, t\right) \text{ , on the boundary surface } s_i.$$

Special cases include the normal derivative of temperature is a function of position only or a function of time only or a constant. If the normal derivative of temperature at the boundary surface vanishes on the boundary surface s_i. This special case is called as the homogeneous boundary condition of second kind.

Also called as the **Neumann boundary condition**, named after Carl Neumann

❖ **Boundary conditions of third kind**

A linear combination of temperature and normal derivative of temperature is prescribed at the boundary surface. For a boundary surface that fits the coordinate surface of the orthogonal coordinate system is given by,

$$k_i \frac{\partial T}{\partial n_i} + h_i T = f_i\left(\overline{r_s}, t\right)$$,on the boundary surface s_i.

A special case is $k_i \frac{\partial T}{\partial n_i} + h_i T = 0$ which is called as boundary condition of third kind also called as the **mixed boundary condition.**

4. Mathematical Methods

❖ **Differential Transform Method**

Differential Transform Method (DTM) is based on the Taylor's series expansion. In 1986, the method was first introduced by Zhou to solve linear and nonlinear initial value problems associated with electrical circuit analysis. The DTM obtains an analytical solution in the form of series.

The basic definitions of differential transform method are introduced as follows,

If a function *u(x,t)* is analytic and continuously differentiable function with respect to time *t* and space variable *x* in the domain of interest, then let

$$U_k(x) = \frac{1}{k!}\left[\frac{\partial^k}{\partial t^k} u(x,t)\right]_{t=0}$$

Where, $U_k(x)$ is the transformed function.

The differential inverse transform of $U_k(x)$ is defined as follows,

$$u(x,t) = \sum_{k=0}^{\infty} U_k(x)\, t^k$$

Then combining the above equations,

$$u(x,t) = \sum_{k=0}^{\infty} \frac{1}{k!} t^k \left[\frac{\partial^k}{\partial t^k} u(x,t)\right]_{t=0}$$

❖ **Finite Difference Method**

- **An explicit method**

Using forward difference in the time domain, the time derivative of temperature *T(x,t)* is given by,

$$\frac{\partial T}{\partial t} = \frac{T_i^{n+1} - T_i^n}{\Delta t} + O(\Delta t)$$

Finite difference expression for partial derivative with respect to the space variable is given as,

$$\frac{\partial T}{\partial x} = \frac{T_{i+1}^n - T_i^n}{(\Delta x)} + O(\Delta x)$$

and

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i-1}^n + T_{i+1}^n - 2T_i^n}{(\Delta x)^2} + O(\Delta x)^2$$

Substituting these values in the one dimensional heat equation, we get the recursive relation as,

$$T_i^{n+1} = rT_{i-1}^n + (1-2r)T_i^n + rT_{i+1}^n \quad , i = 1, 2, ...N-1, n = 0, 1, 2, ...$$

where, $r = \frac{\alpha \Delta t}{(\Delta x)^2}$ and truncation error of order $O(\Delta t) + O(\Delta x)^2$

The boundary conditions involving derivatives which should be expressed in finite

The entire set of equations are stable for $0 < r \equiv \frac{\alpha \Delta t}{(\Delta x)^2} \leq \frac{1}{2}$.

- **Crank Nicolson implicit method**

The Crank Nicolson finite difference method was invented by John Crank and Phyllis Nicolson. They originally applied to the heat equation and they approximated the solution of the heat equation on some finite grid by approximating the derivatives in space variable *x* and time by finite difference.

The one dimensional heat equation is approximated numerically by,

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \frac{1}{2}\alpha \left[\frac{T_{i-1}^{n+1} + T_{i+1}^{n+1} - 2T_i^{n+1}}{(\Delta x)^2} + \frac{T_{i-1}^n + T_{i+1}^n - 2T_i^n}{(\Delta x)^2} \right]$$

The above finite difference equations are rearranged in the following form,

$$-rT_{i-1}^{n+1} + (2+2r)T_{i}^{n+1} - rT_{i+1}^{n+1} = rT_{i-1}^{n} + (2-2r)T_{i}^{n} + rT_{i-1}^{n}, i = 0,1,...,N$$

This relation is called as Clank-Nicolson algorithm and it requires a simultaneous solution of all the equations at each time step.

❖ **Integral Transform Method**

In solving the transient heat conduction problems it is useful to apply Laplace transform to remove time variable from the partial differential equation. However in many problems it is convenient to apply an integral transformation that removes the space variable from the partial differential equation. The integral transform technique is especially attractive for transient and steady state heat conduction problems in that it treats all the space variables in same manner and has no inversion difficulty.

We define the integral transform as,

$$\bar{T}(\beta_m, t) = \int_{x=0}^{L} K(\beta_m, x').T(x', t)dx'$$

and the Inversion formula as,

$$T(x,t) \sum_{m=1}^{\infty} K(\beta_m, x).\bar{T}(\beta_m, x)$$

where., $K(\beta_m, x)$ is the kernel and can be designed according to the boundary conditions of the given problem.

❖ **Finite Element Method**

Finite element method (FEM) is a numerical method for solving a differential or integral equation. It has been applied to a number of physical problems, where the governing differential equations are available. The method essentially consists of assuming the piecewise continuous function for the solution and obtaining the parameters of the functions in a manner that reduces the error in the solution method is illustrated with the help of the plane stress and plane strain formulation.

Following are the steps of the finite element formulation:

(i) Preprocessing that includes mesh generation.

(ii) Obtaining the assembled system of equations, for which the elemental matrices and vectors need to be evaluated

(iii) Applying the boundary conditions

(iv) Solving the linear system of equations and

(v) Post-processing. The time-dependent problems are solved by treating the derivative with time by the finite difference approximation. The derivatives with respect to spatial variables are tackled in the usual way of FEM.

5. Review of Literature

In 2021, Amiri Delouei, *et al.* [1], different existing analytical solutions for heat conduction in multi-layer and composite materials are reviewed and classified in rectangular, cylindrical, spherical, and conical coordinates. Applied boundary conditions, internal heat source, and thermal contact resistance as the most critical parameters in the solution complexity investigated in the literature, are discussed and summarized in different tables.

In 2020, Aysegul Ozgur *et al*. [2] proposed a numerical method for solving elastic stress problems in hollow discs made of functionally graded materials (FGM) that are exposed to linearly increasing temperature dispersion. The FGM disk's modulus of elasticity and coefficient of thermal expansion are assumed to change in various ways along the radial direction.

In 2019, The net residual stresses in the films of American Superconductor tape were investigated using a displacement-energy model (DEM) solution approach by Stephen Ogbonna Mbam *et al*. [3]. The DEM solution method was created to forecast the thermal mismatch and inherent film stresses in coated conductor films.

In 2018, Jiangbo Luo *et al*. [4] established general theoretical models for elastic and elastic-plastic deformation in multilayer films with void regions filled with other solids or gases, and investigated the difference in critical temperature for the film as it transitioned from elastic to plastic deformation.

In 2016, Marianito R. Rodrigo and Annette L. Worthy [5], considered a one-dimensional multilayer diffusion problem subject to nonhomogeneous boundary conditions. Unlike previous results that used a separation of variables technique to solve such problems with homogeneous boundary conditions, here we use a Laplace transform approach.

In 2016, E.J. Carr, I.W. Turner [6] , considered a diffusion in a composite slab consisting of a large number of layers provides an ideal prototype problem for developing and analyzing

two-scale modelling approaches for heterogeneous media. Numerous analytical techniques have been proposed for solving the transient diffusion equation in a one-dimensional composite slab consisting of an arbitrary number of layers.

In 2011, S. McGinty, S. McKee, R.M. Wadsworth, C. McCormick [7] , considered a family of mathematical models to describe the elution of drug from polymer-coated stents into the arterial wall. The models include the polymer layer, the media, the adventitia, a possible topcoat polymer layer and atherosclerotic plaque. Also investigated the relative importance of transmural convection, diffusion and drug-dependent parameters in drug delivery and deposition.

In 2011, R. Pasupuleti, Y. Wang, I. Shabalin, L.Y. Li, Z. Liu, S. Grove [8], presented a numerical investigation on the moisture diffusion taking place in multilayer woven fabric composites.. Using finite element analysis methods, the microscopic heterogeneity of RUC is described in terms of the tow size, tow cross-section shape and tow weaving configuration of fabrics.

In 2011, S. Mitragotri, Y.G. Anissimov [9] , provided an overview of various modeling approaches with respect to their advantages, limitations and future prospects.

In 2010, Le-Chung Shiau, Shih-Yao Kuo, Cheng-Yuan Chen [10], studied thermal buckling behavior of composite laminated plates was studied by making the use of finite element method.

In 2009, G. Liu, B.C. Si [11], presented an analytical solution for either perfectly mixed or non-mixed non-steady-state (NSS) chamber systems with a depth-dependent gas production term.

In 2008, Kulkarni V.S. and Deshmukh K.C. [12], determined the unknown temperature and thermal stresses on the upper surface of a thick circular plate. The results for displacement and stresses have been computed numerically and illustrated graphically.

In 2005 , L. Simon, N.W. Loney [13] , used Laplace transform to solve a mathematical model developed for percutaneous drug absorption. This model includes application and

removal of the vehicle from the skin. A system of two linear partial differential equations was solved for the application period.

In 2002 , M.A. Sales-Cruz, E.S. Pérez-Cisneros, J.A. Ochoa-Tapia [14] , developed an analytic solution for the dynamic diffusive transport in a multilayer system. The partial differential equations of the mode\ are subjected to boundary conditions, which may be chosen as any function of the time.

In 2000, .F. de Monte [15], analyzed the transient response of one-dimensional multilayered composite conducting slabs to sudden variations of the temperature of the surrounding fluid. The solution is obtained applying the method of separation of variables to the heat conduction partial differential equation. In separating the variables, the thermal diffusivity is retained on the side of the modified heat conduction equation where the time-dependent function is collected.

In 2000, M.F. Abdul Azeez, A.F. Vakakis [16], presented an analytical/numerical method for solving the problem of non-stationary heat diffusion in multilayered slabs. This is an extension of previous methods that have been used to solve transient heat diffusion problems in one-dimension.

In 1998 , C. Liu, W.P. Ball [17] , presented a new analytical solution for solute diffusion in a semi- infinite two-layer porous medium for arbitrary boundary and initial conditions. The solution was obtained by using the Green's function approach in the Laplace domain with the application of the binomial theorem to facilitate inversion back to the real time domain. Results based on this solution were found to be simple both in form and ease of calculation and to be in good agreement with those obtained using numerical calculations based on the Crank-Nicolson finite difference method. Applications of the solution are presented in the context of a contaminated groundwater aquitard to demonstrate how different boundary and initial conditions can greatly affect the contamination and decontamination of porous media, and to illustrate how diffusion modeling might be used in a forensic sense.

Objectives of proposed research:

1) To study basic concepts of heat transfer in composite medium.
2) To study some methods to solve partial differential equations for composite medium.
3) To study the analytical and numerical methods.
4) To compare the solution of the partial differential equations by analytical and numerical methods.
5) To analyze the development in results for partial differential equations.
6) To study recent applications of partial differential equations.
7) Hence, in the present work, we will try to develop the new analytical results and new iterative techniques for partial differential equation and to obtain their solution. These will represent graphically by Mathematica, MATLAB, Python, Scilab and Mathcad.

Research Methodology:

The following steps will be including in the methodology:
1) To refer the relevant reference books on partial differential equations for composite medium.
2) To study Mathematica, MATLAB, Python, Scilab, Mathcad softwares.
3) To study analytical solution of partial differential equations for composite medium.
4) To study Numerical methods for obtaining approximate solutions of Partial differential equations.
5) To discuss the stability and convergence of Numerical methods.
6) To represent Numerical solutions of partial differential equations graphically by Mathematica, MATLAB and discuss their nature.
7) Comparison of solution to validate numerical solution.

Plan of work:

Sr. No.	Period	Plan of work	Targets to be Achieved
1	First year	Study of background information relevant to the research issue	Excellent understanding of the subject and well-organized coursework.
2	Second year	Collecting and analysing research articles.	Attempt to obtain new results based on existing work and submit some papers.
3	Third year	Publishing some papers and writing of the thesis.	Some more papers and thesis submission.

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